Electronic Supplementary Material (ESI) for New Journal of Chemistry.


***Supporting information***

# Theoretical Study of the Electronic Structure of the Complexes of Gold, Silver, and Copper Mono- and Bimetallic Nanoclusters Decorated on Graphitic Carbon Nitride (g-$C_3N_4$): DFT and TD-DFT Study of Photocatalytic Activity

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***Summary of content:*** *This Supporting Information file contains 21 Figures presented in 21 pages.*

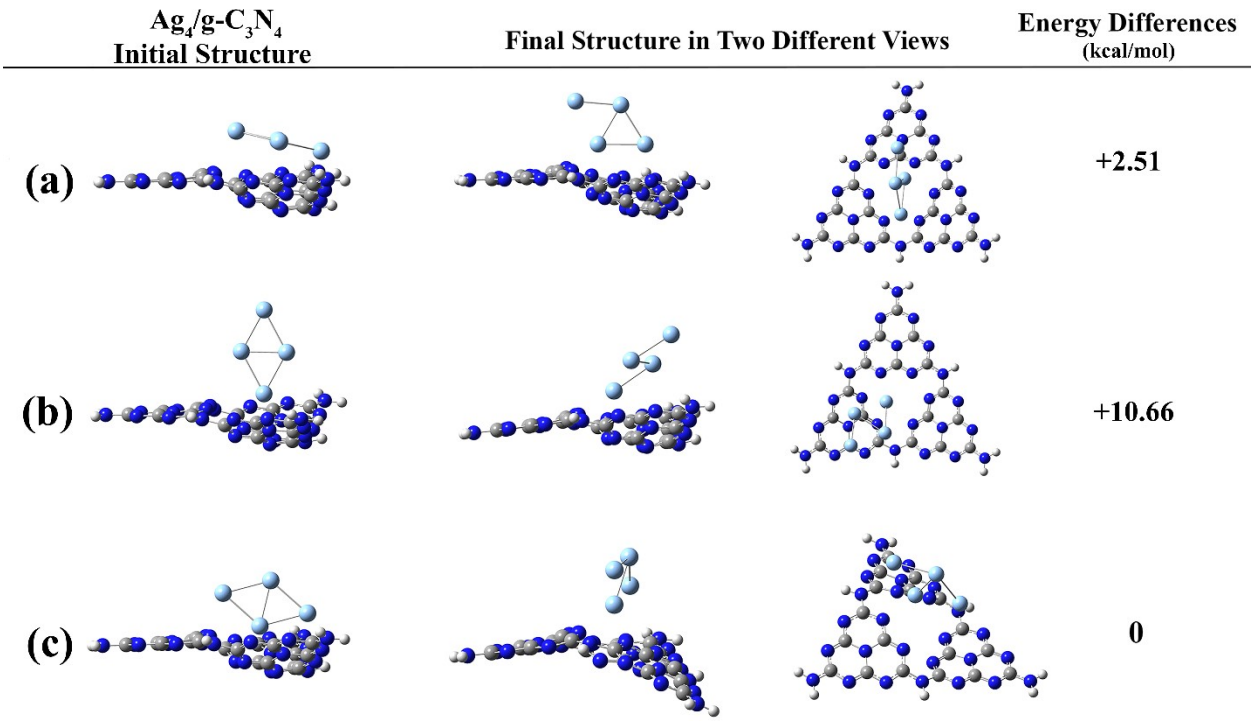


**Fig. S1.** The initial and optimized (two views) geometries of $Ag_4/g\text{-}C_3N_4$ complexes and their energies relative to the most stable structure.

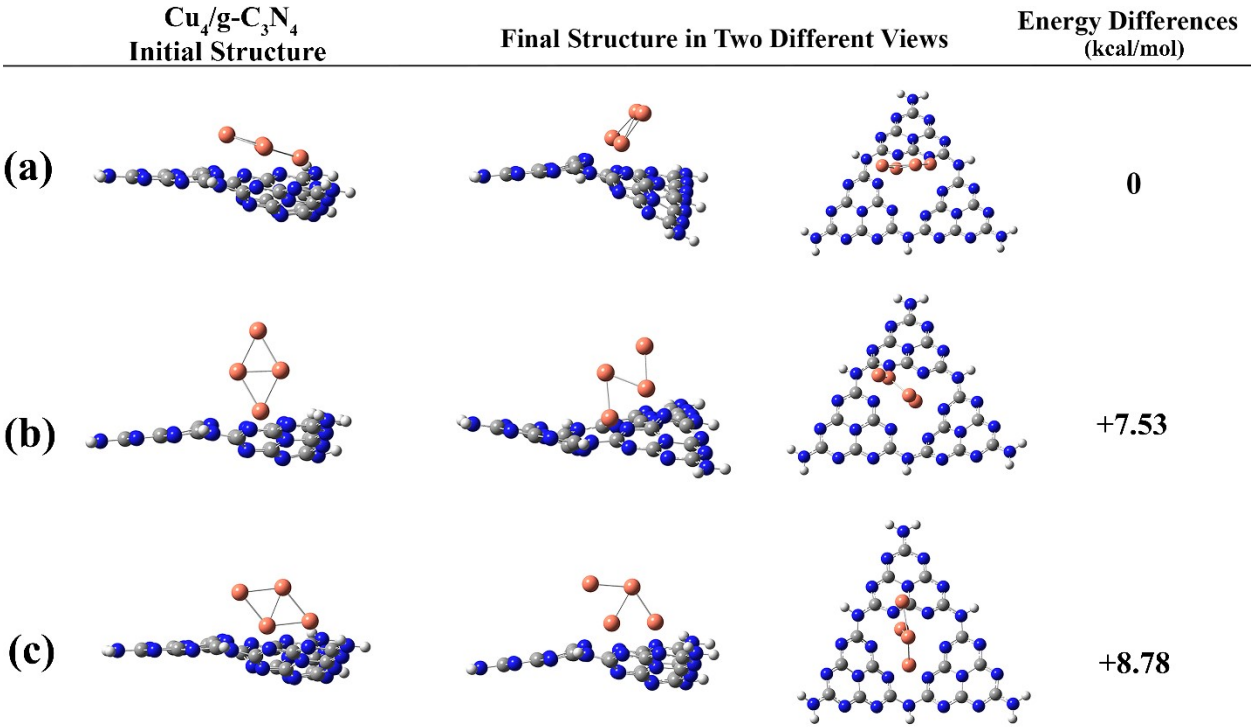


**Fig. S2.** The initial and optimized (two views) geometries of $Cu_4/g\text{-}C_3N_4$ complexes and their energies relative to the most stable structure.

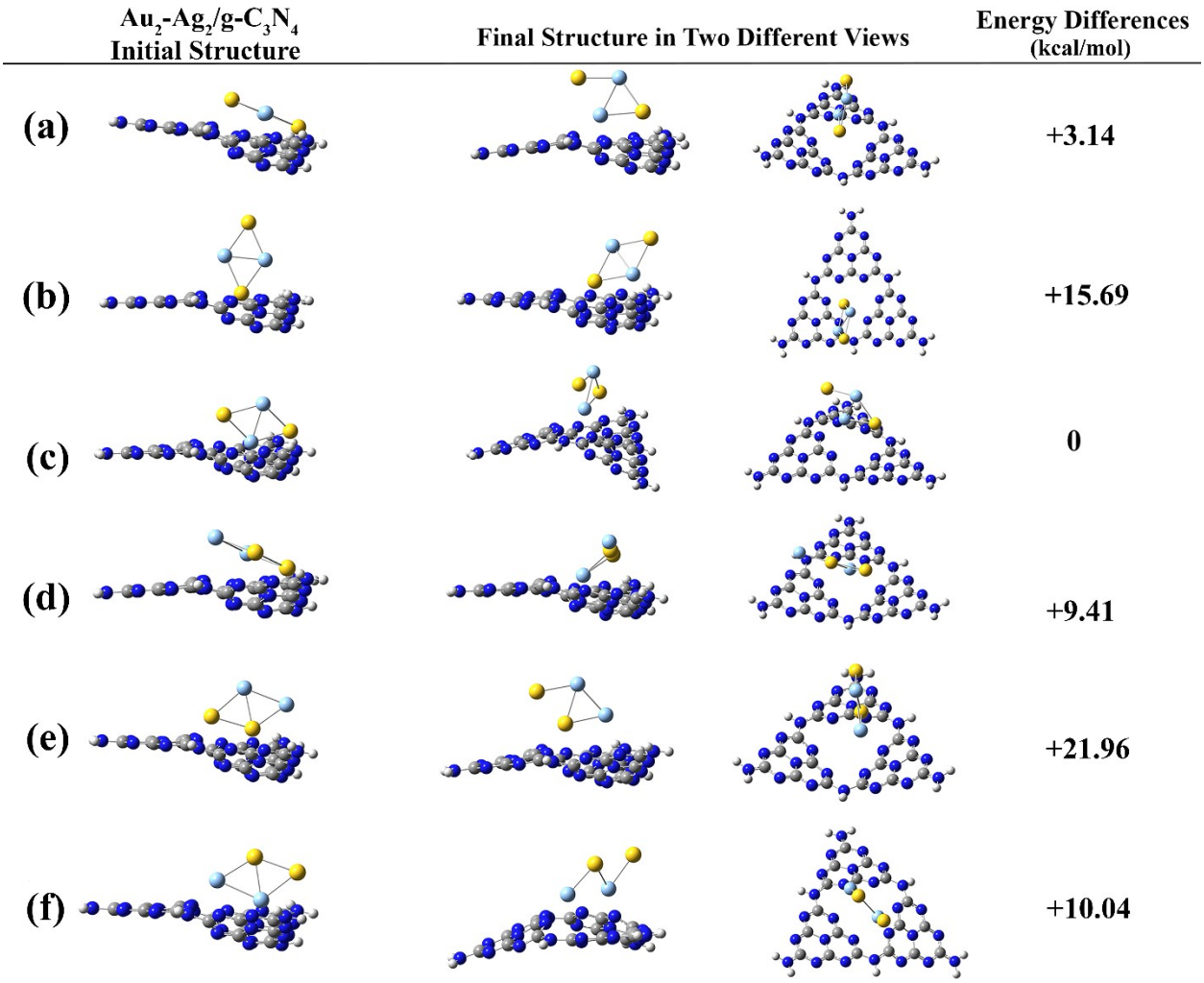


**Fig. S3.** The initial and optimized (two views) geometries of $Au_2$-$Ag_2$/g-$C_3N_4$ complexes and their energies relative to the most stable structure.

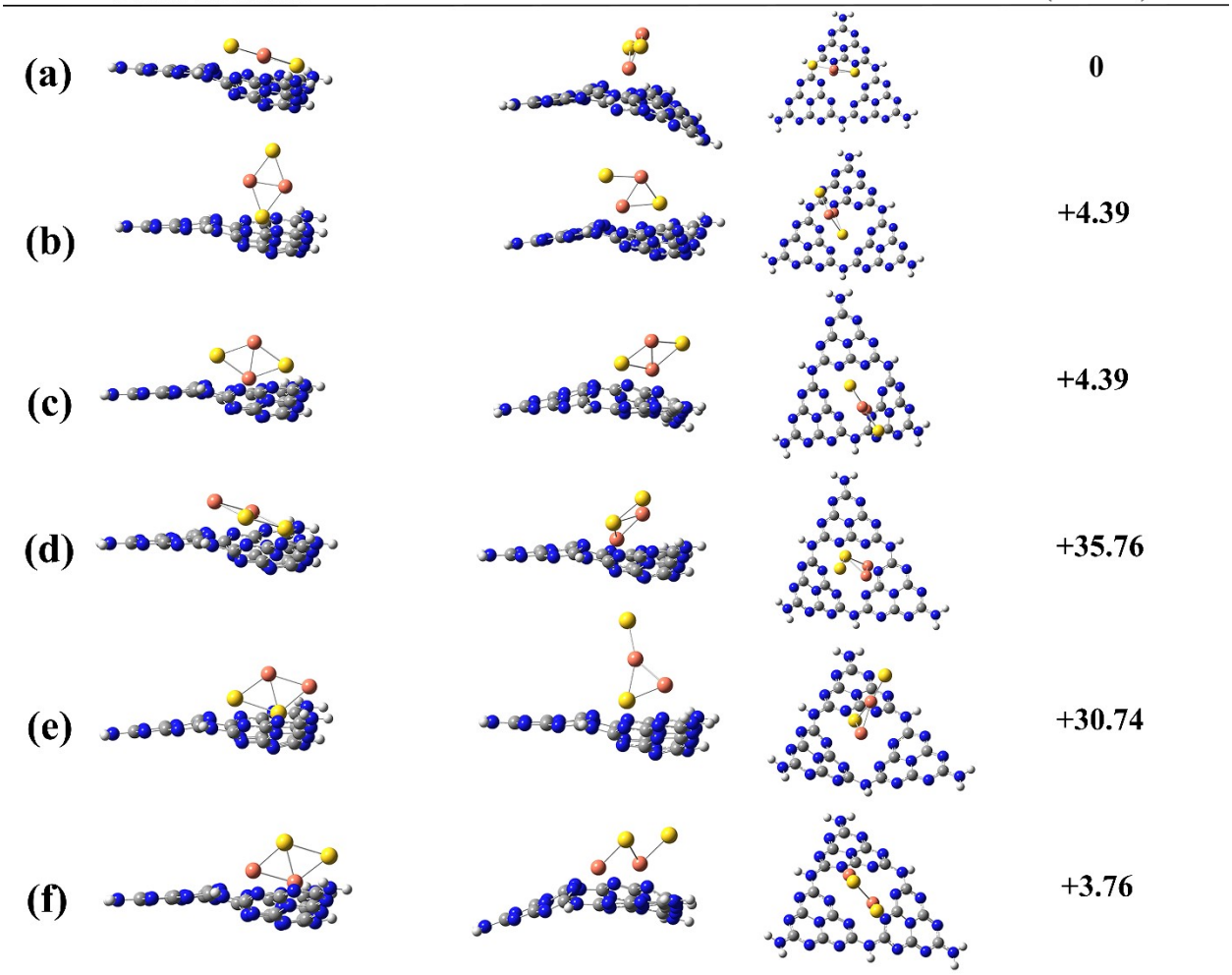


**Fig. S4.** The initial and optimized (two views) geometries of $Au_2$-$Cu_2$/g-$C_3N_4$ complexes and their energies relative to the most stable structure.

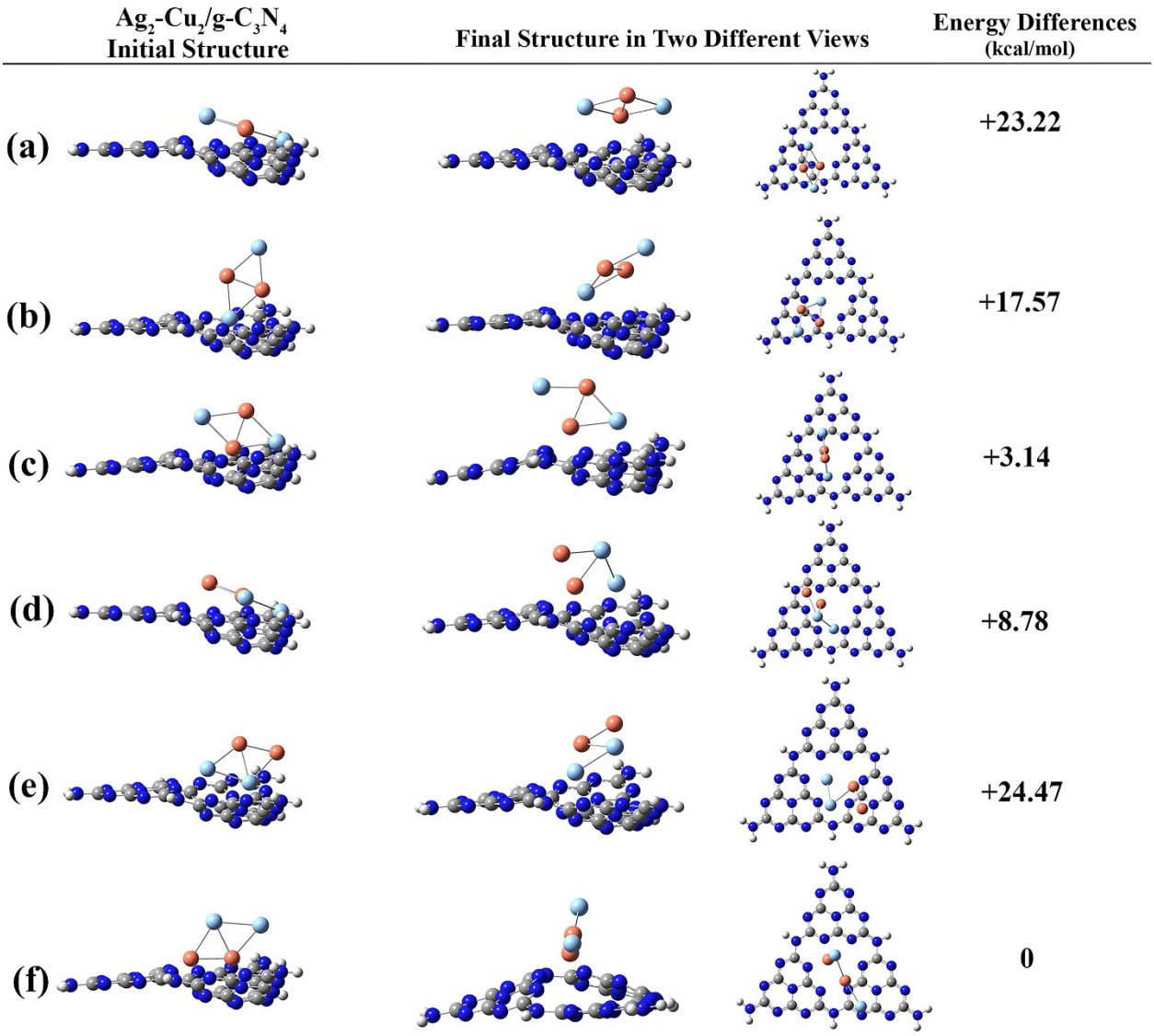


**Fig. S5.** The initial and optimized (two views) geometries of $Ag_2$-$Cu_2$/g-$C_3N_4$ complexes and their energies relative to the most stable structure.

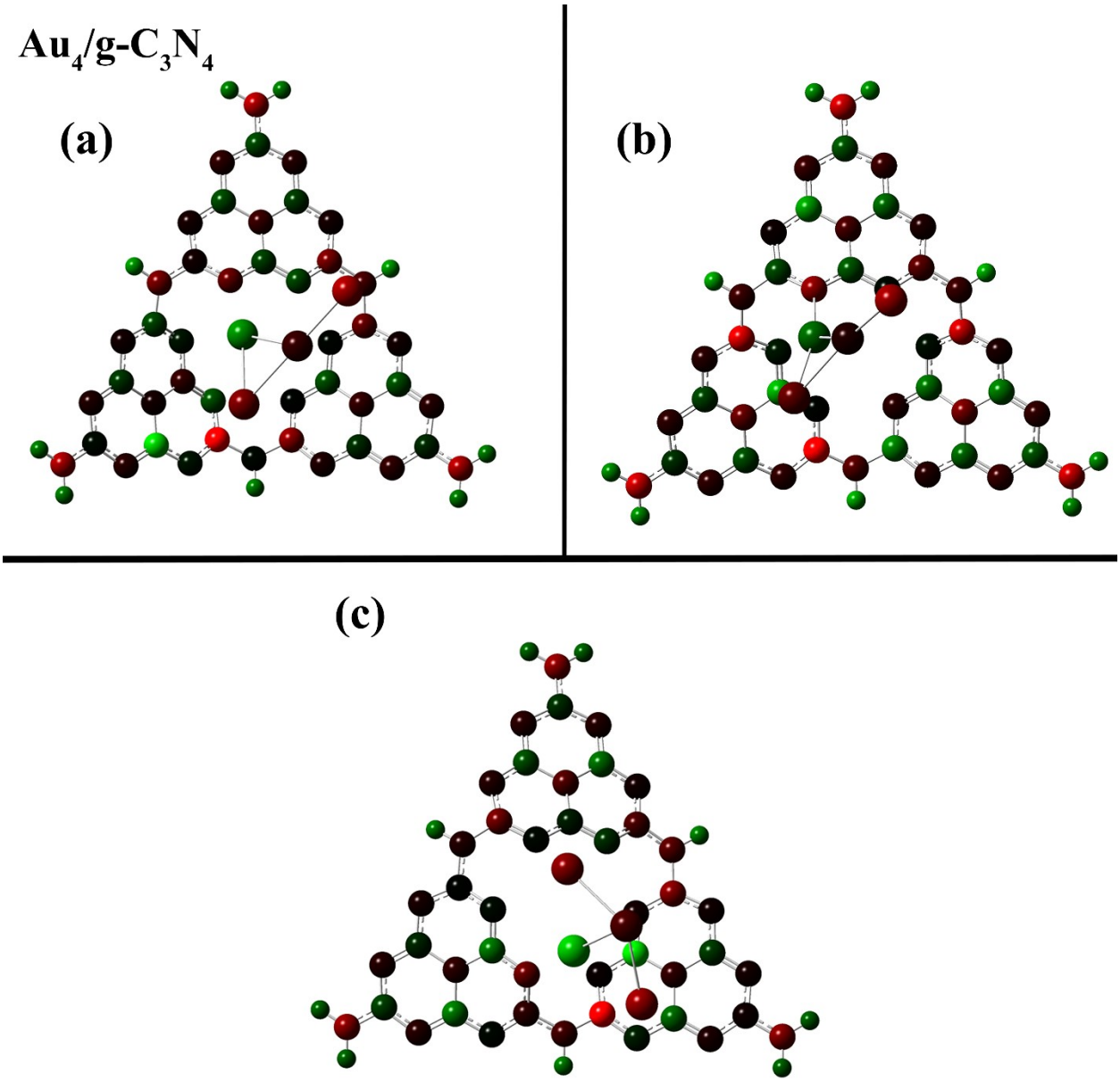


**Fig. S6.** The colored representation of the partial charges of three optimized $Au_4/g\text{-}C_3N_4$ complexes.

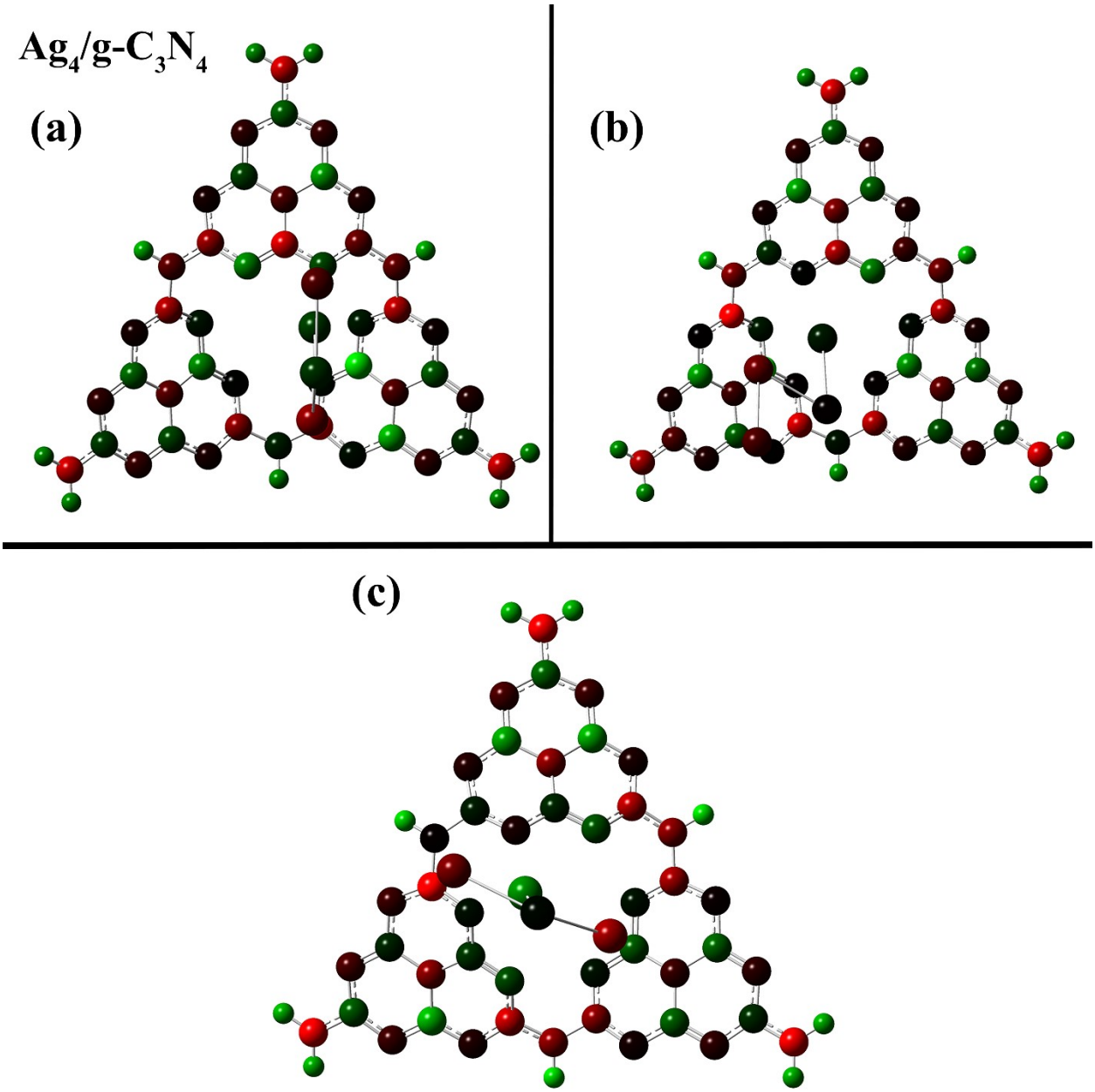


**Fig. S7.** The colored representation of the partial charges of three optimized $Ag_4/g\text{-}C_3N_4$ complexes.

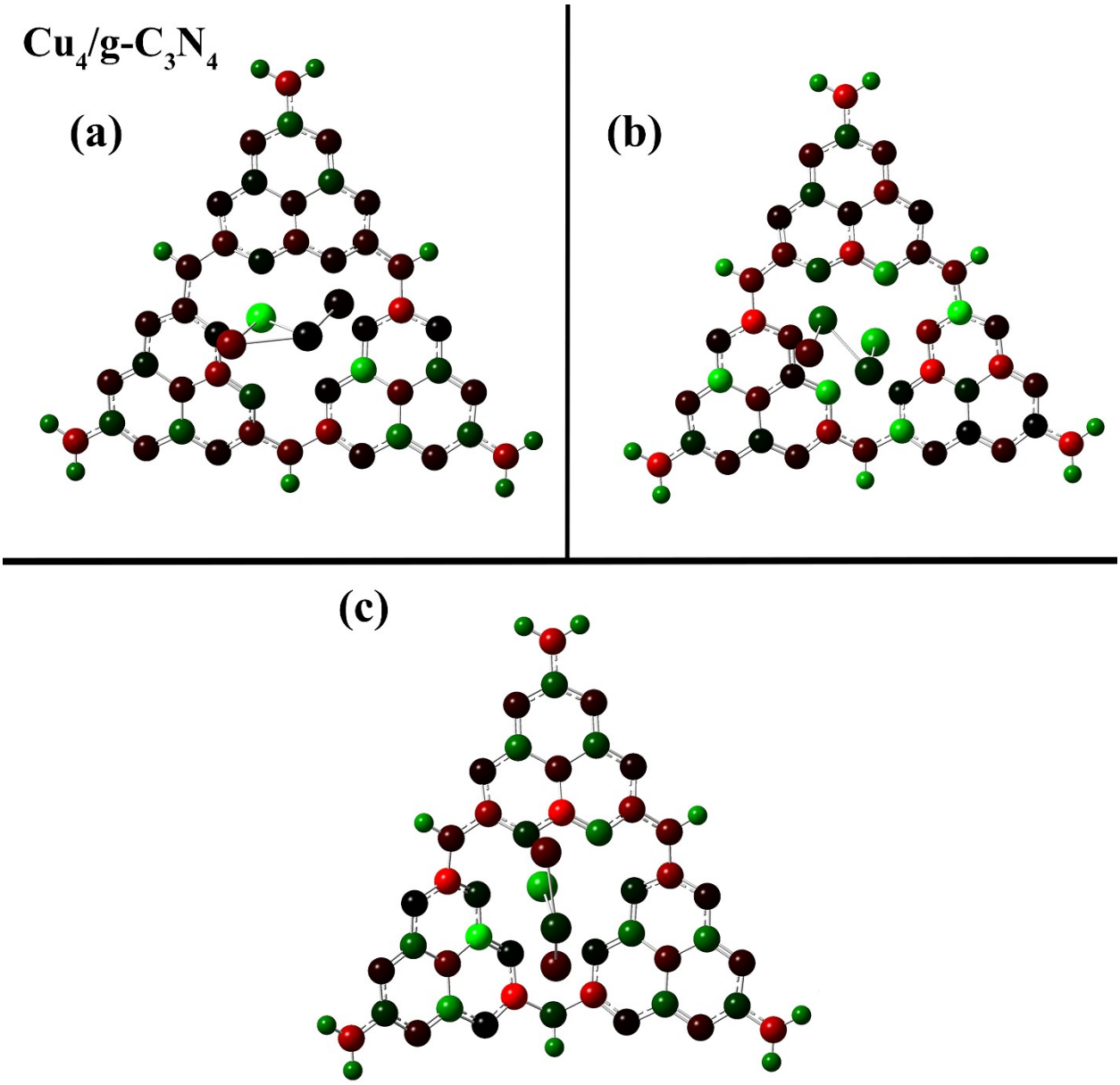


**Fig. S8.** The colored representation of the partial charges of three optimized $Cu_4/g\text{-}C_3N_4$ complexes.

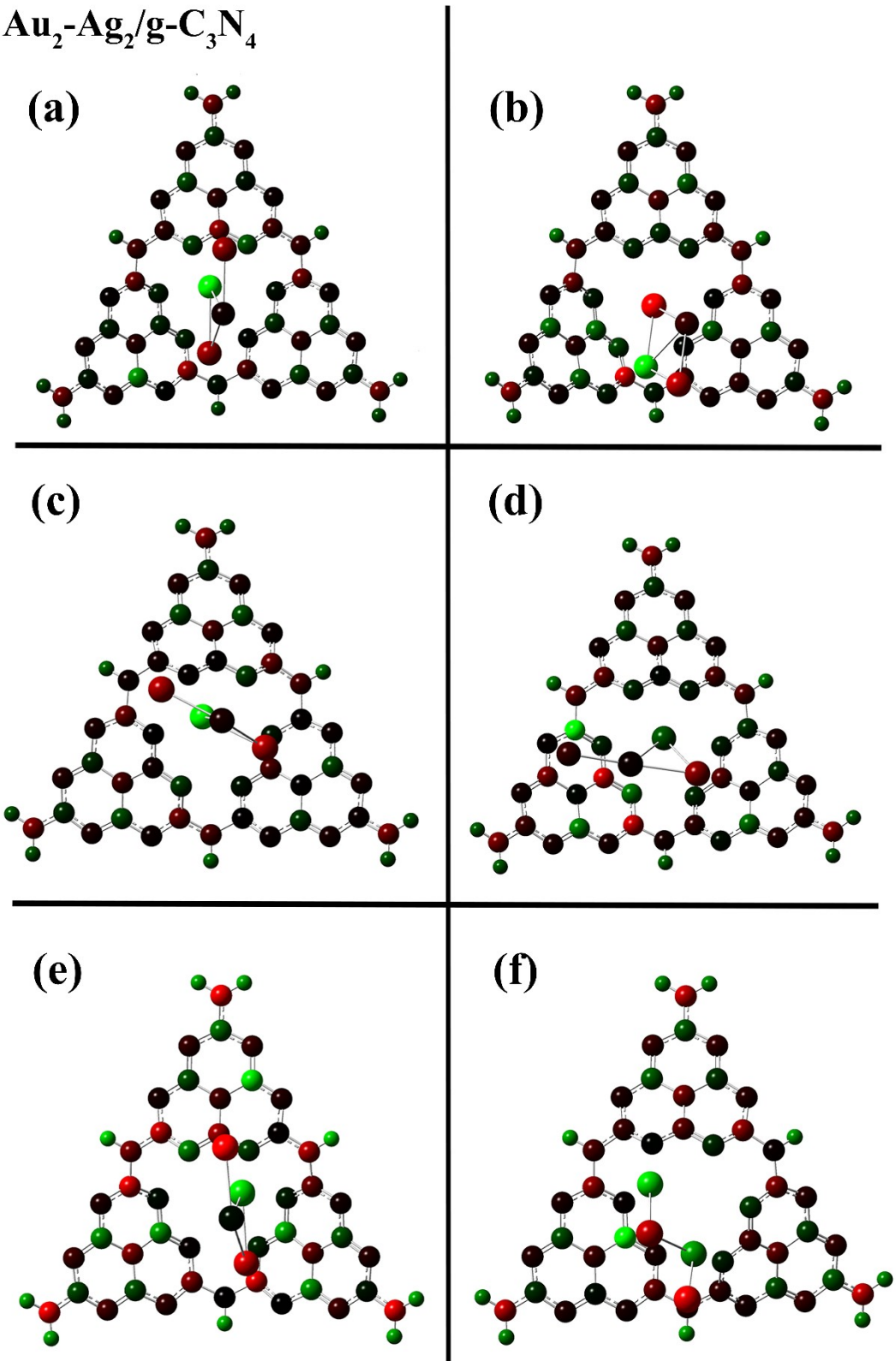


**Fig. S9.** The colored representation of the partial charges of six optimized $Au_2$-$Ag_2$/g-$C_3N_4$ complexes.

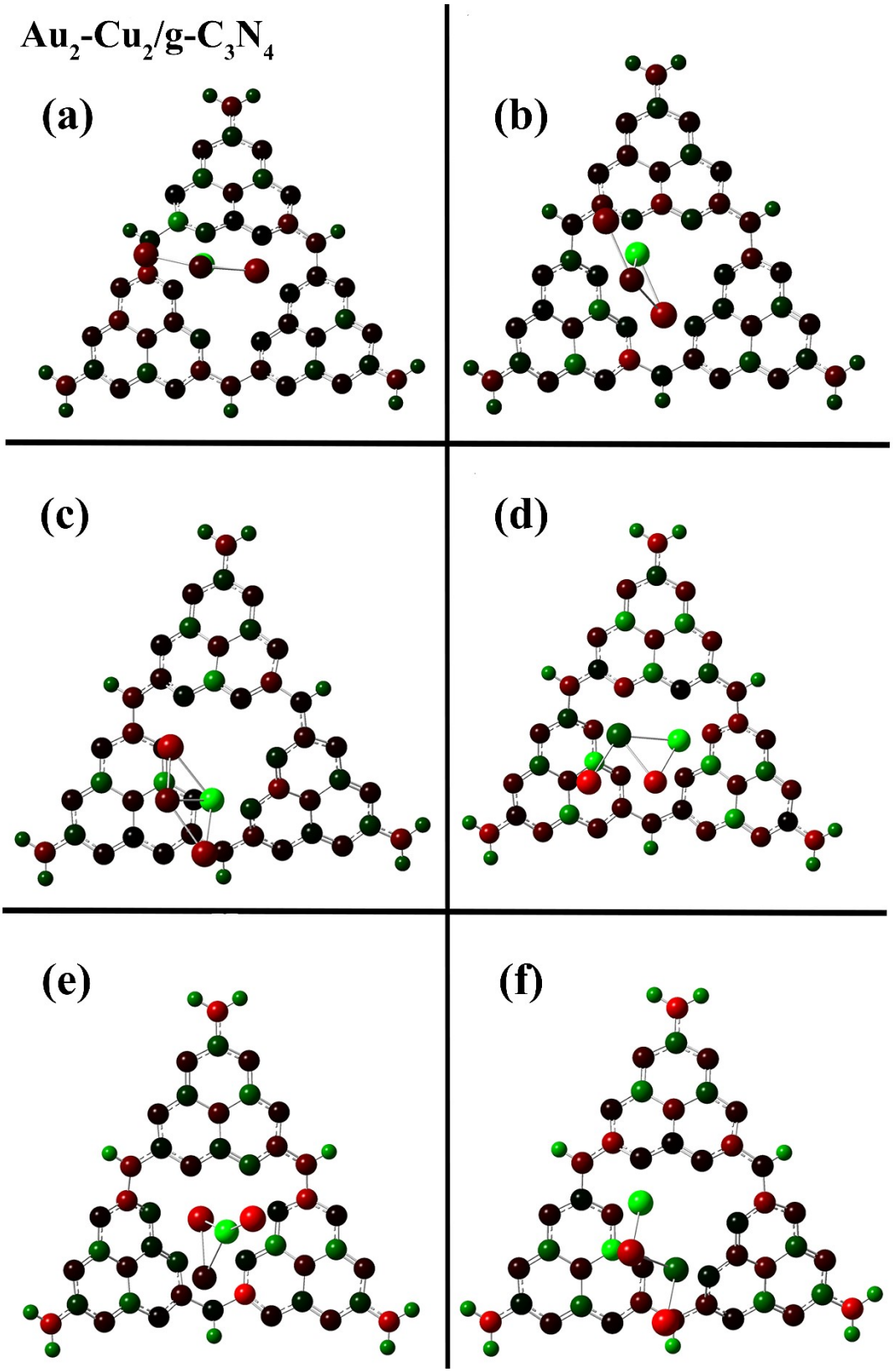


**Fig. S10.** The colored representation of the partial charges of six optimized $Au_2$-$Cu_2$/g-$C_3N_4$ complexes.

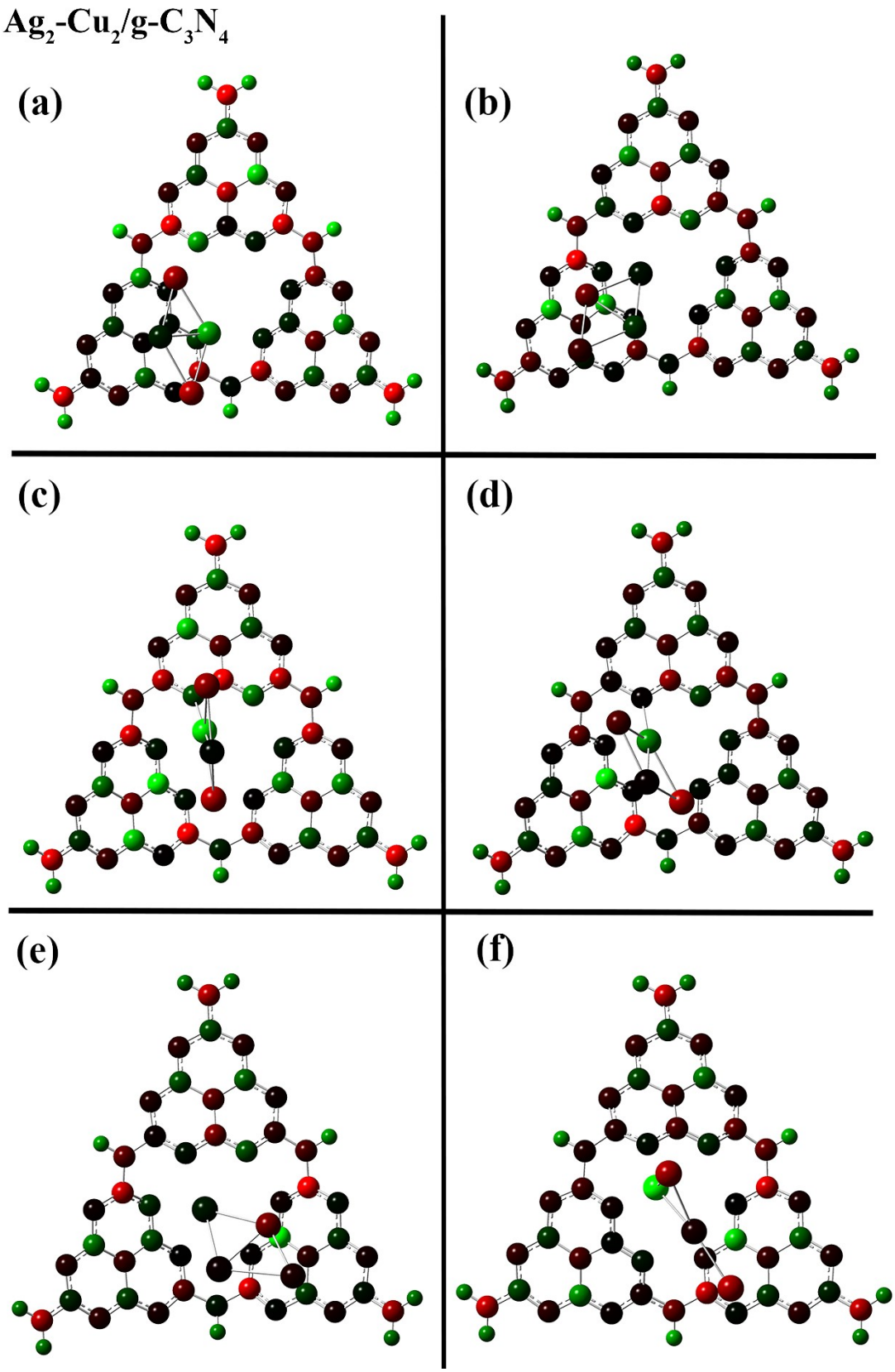


**Fig. S11.** The colored representation of the partial charges of six optimized $Ag_2$-$Cu_2$/g-$C_3N_4$ complexes.

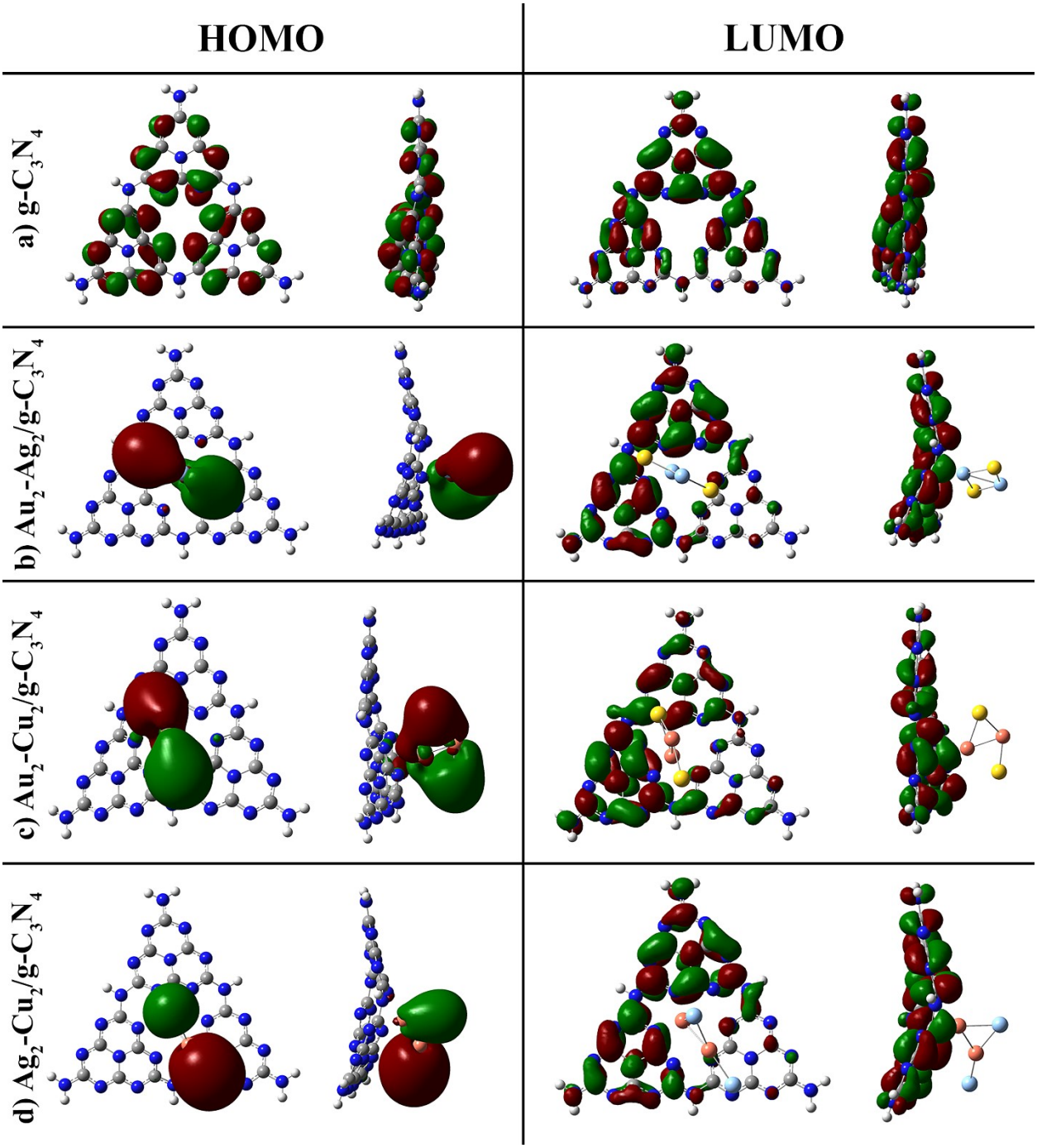


**Fig. S12.** Two views of the HOMO and LUMO of (a) the bare g-$C_3N_4$ and the most stable (b) $Au_2$-$Ag_2$, (c) $Au_2$-$Cu_2$, and (d) $Ag_2$-$Cu_2$/g-$C_3N_4$ complexes.

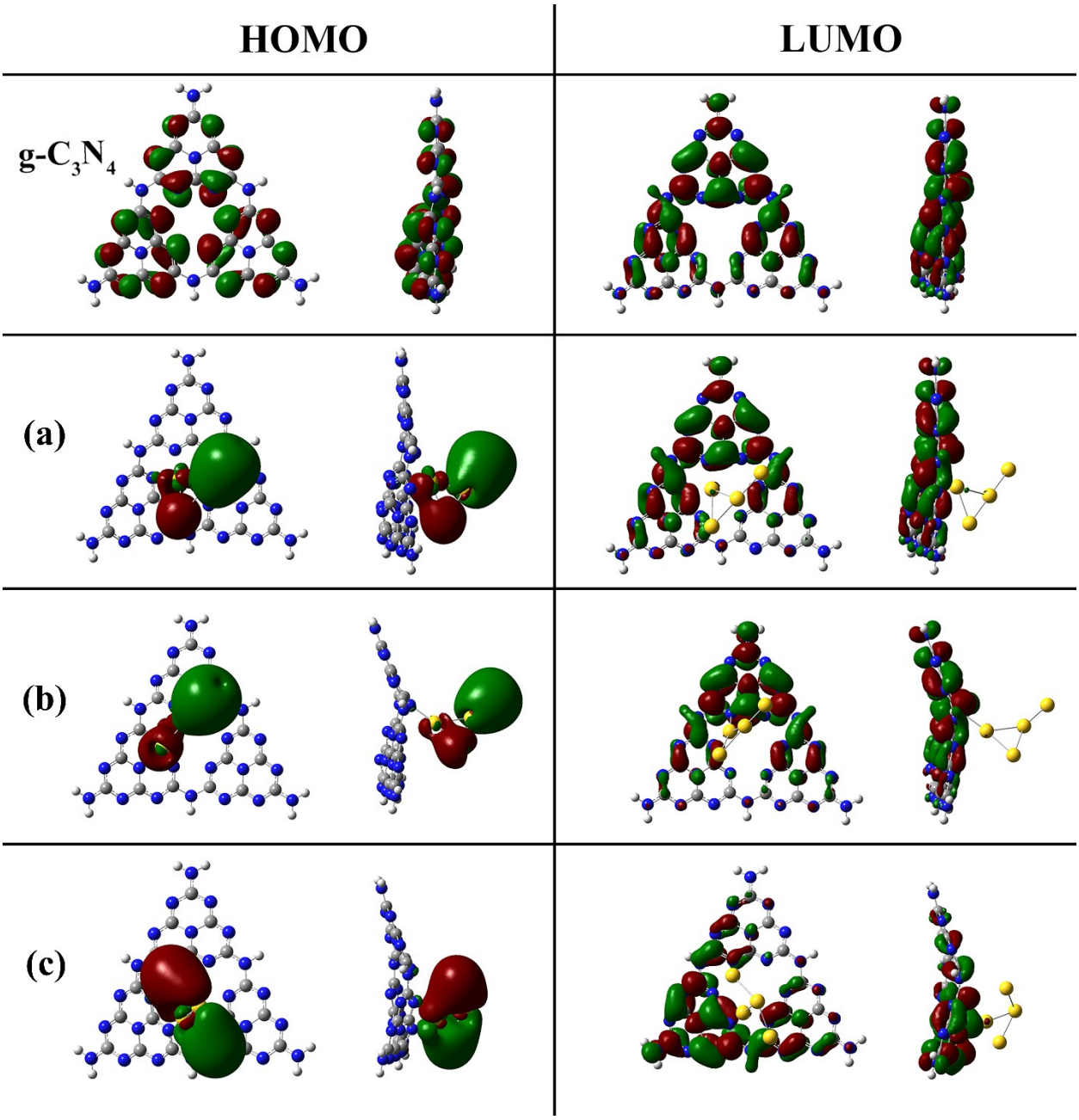


**Fig. S13.** Two views of the HOMO and LUMO for the bare g-$C_3N_4$ and three optimized $Au_4$/g-$C_3N_4$ complexes.

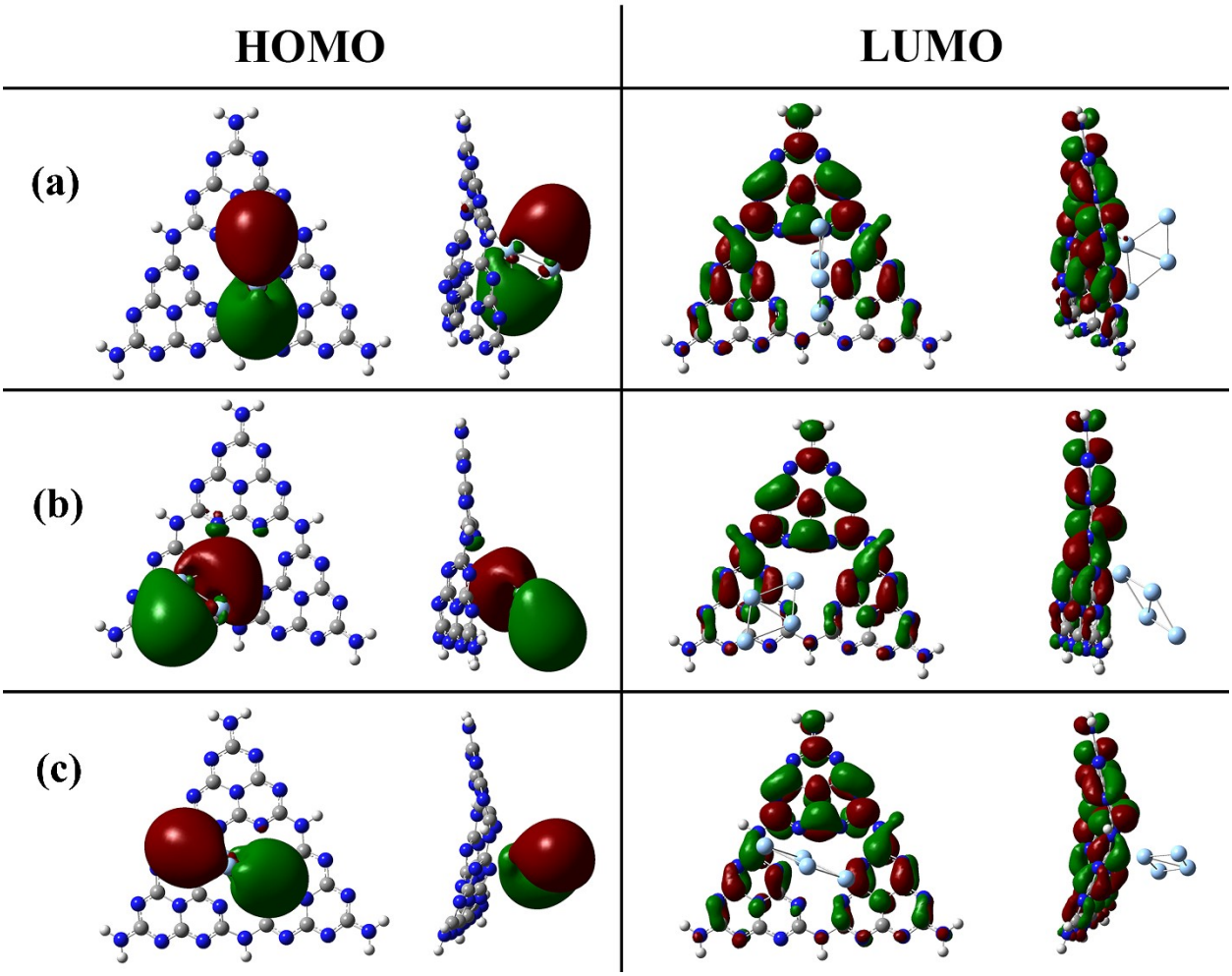


**Fig. S14.** Two views of the HOMO and LUMO for three optimized $Ag_4$/g-$C_3N_4$ complexes.

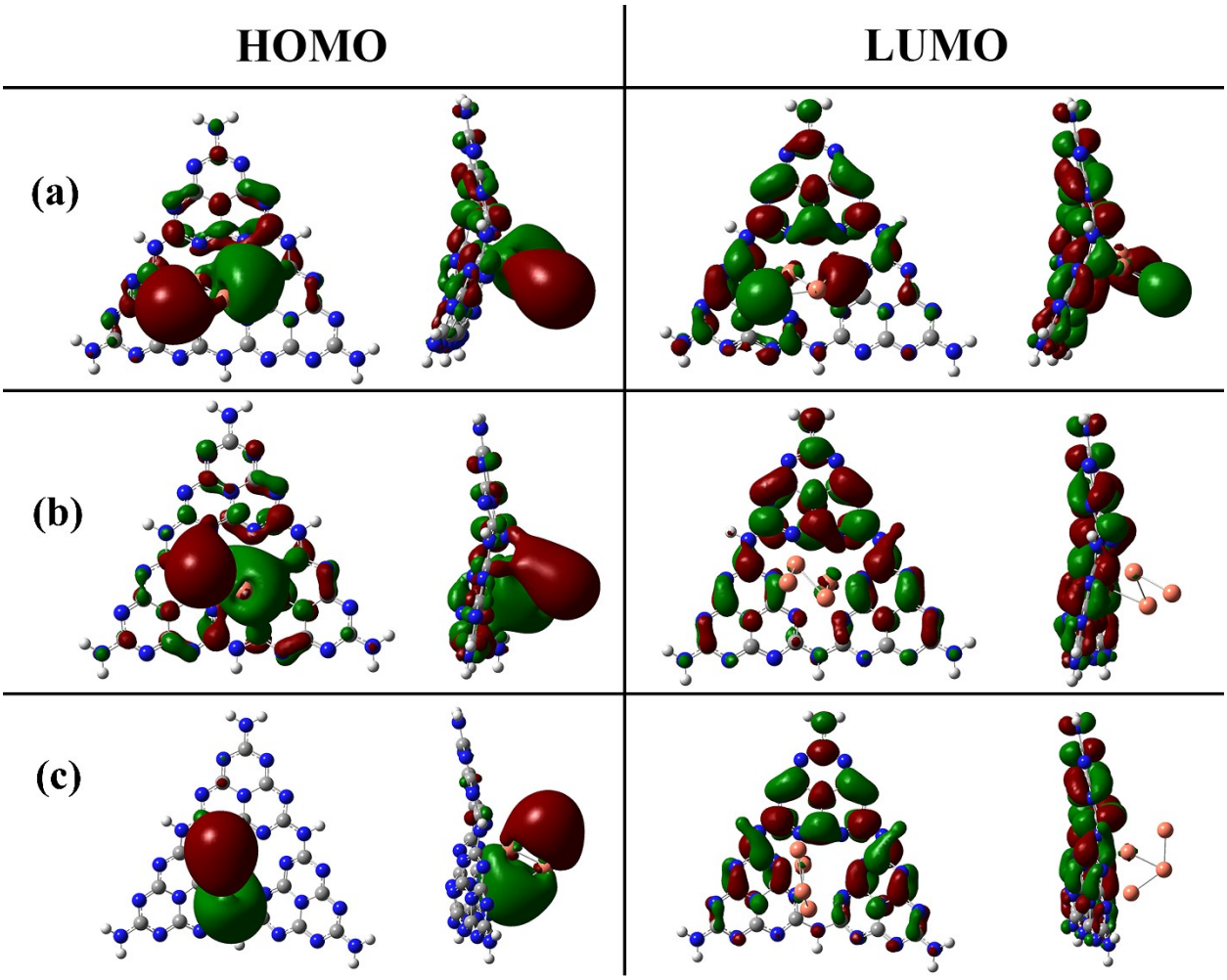


**Fig. S15**. Two views of the HOMO and LUMO for three optimized $Cu_4$/g-$C_3N_4$ complexes.

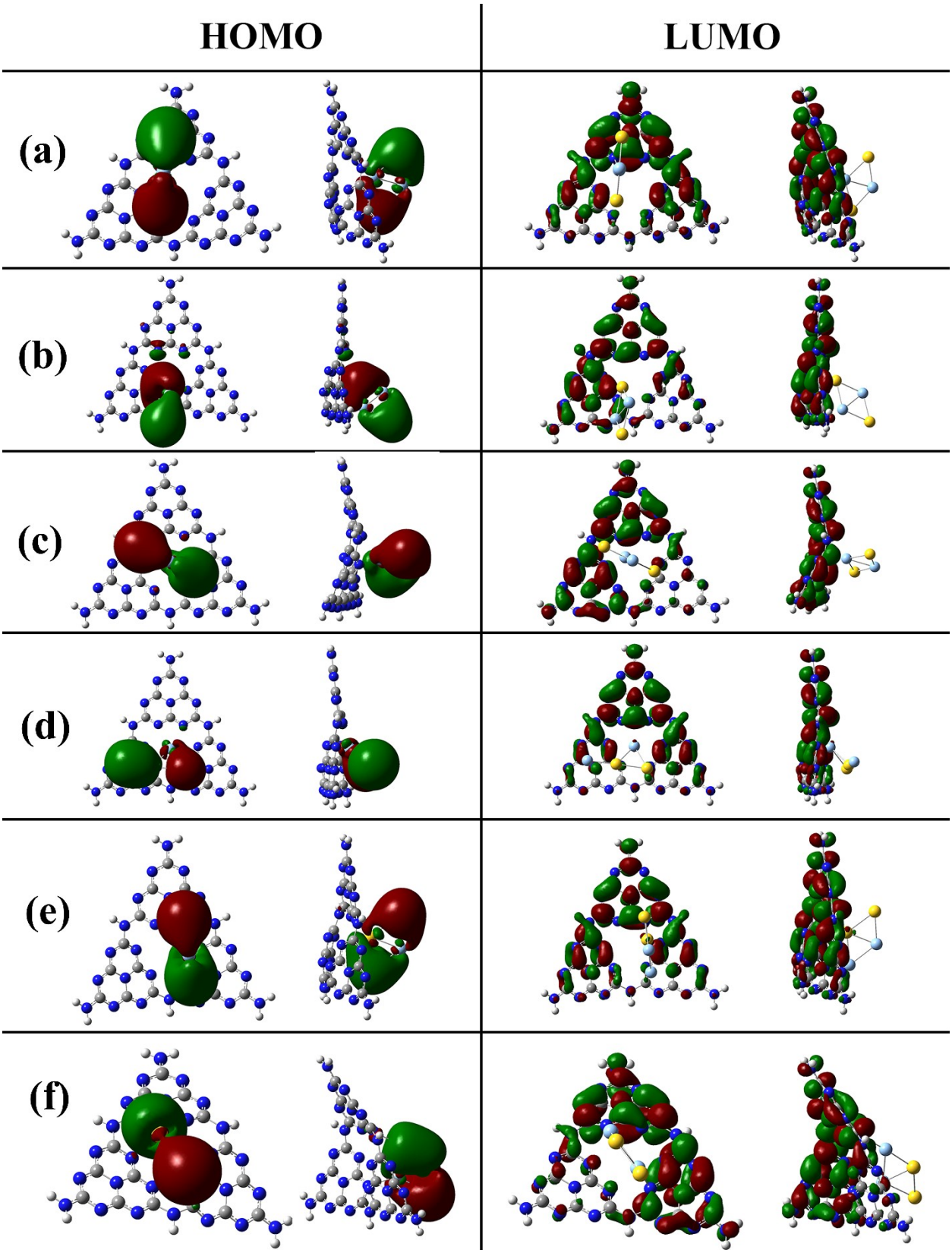


**Fig. S16**. Two views of the HOMO and LUMO for six optimized $Au_2$-$Ag_2$/g-$C_3N_4$ complexes.

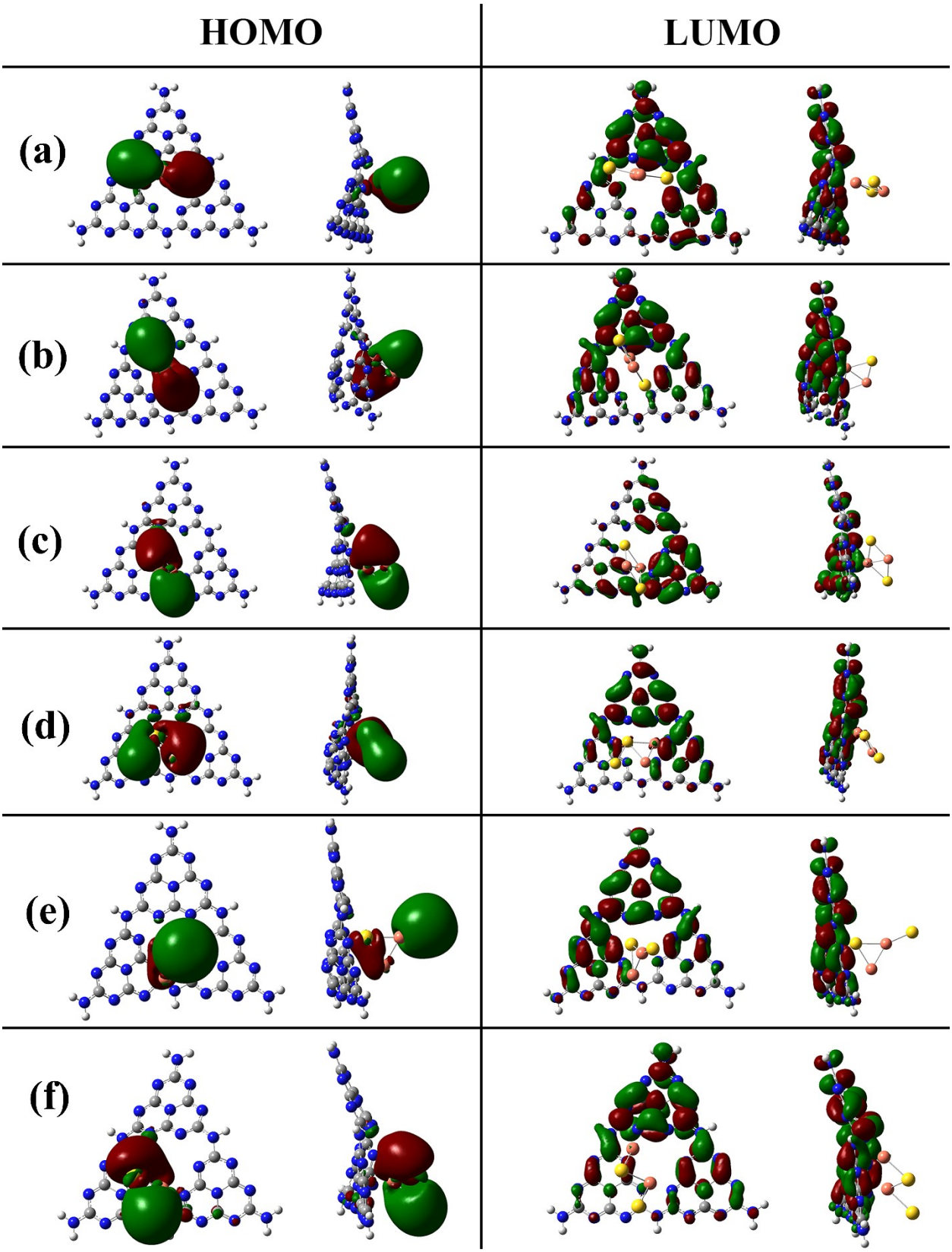


**Fig. S17.** Two views of the HOMO and LUMO for six optimized $Au_2$-$Cu_2$/g-$C_3N_4$ complexes.

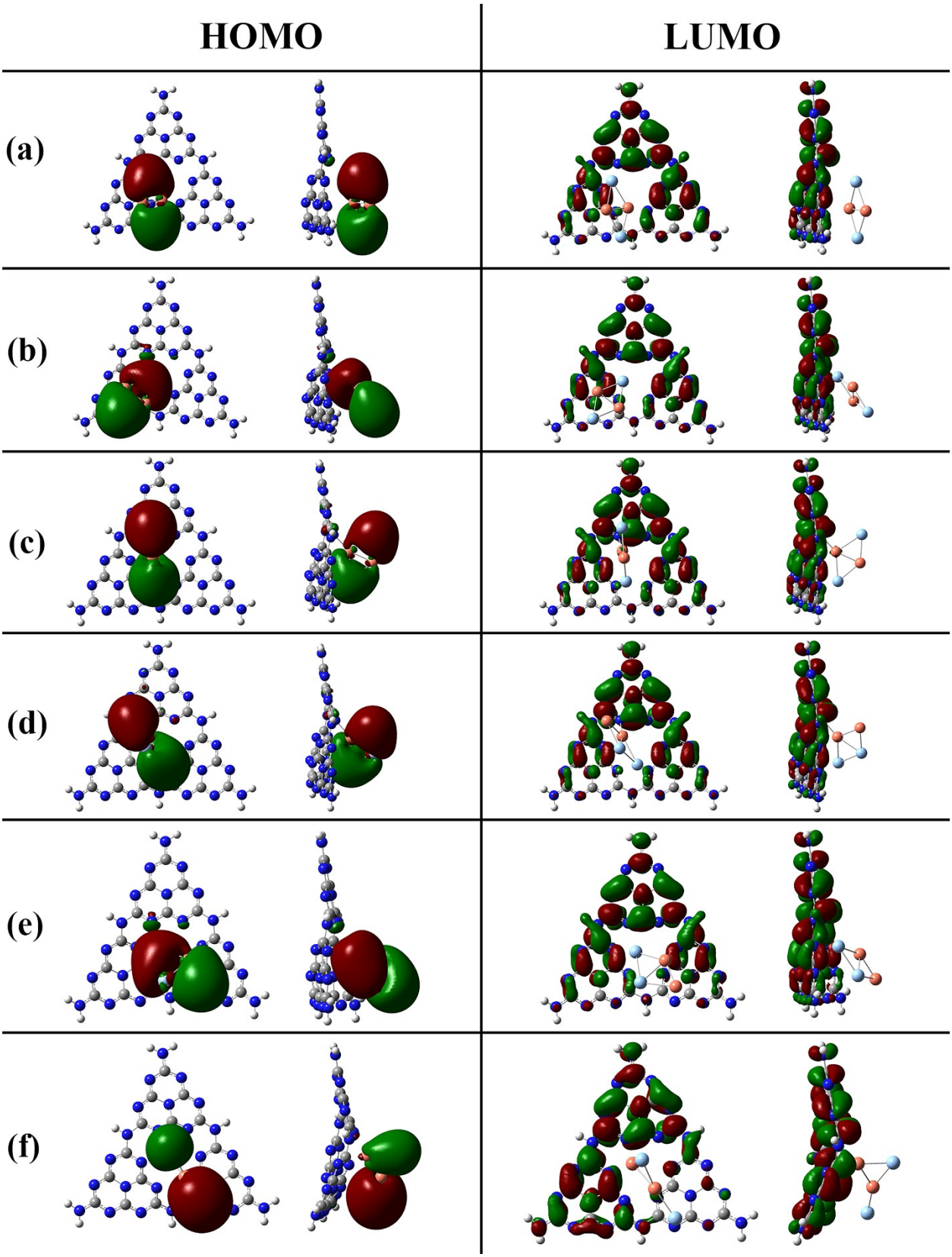


**Fig. S18**. Two views of the HOMO and LUMO for six optimized $Ag_2$-$Cu_2$/g-$C_3N_4$ complexes.

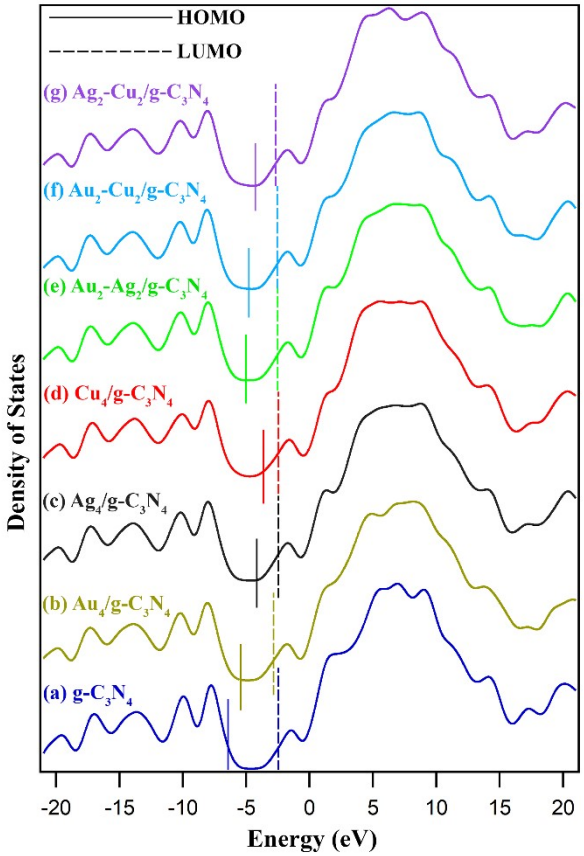


**Fig. S19.** The comparison of the (a) TDOS diagram for the bare g-$C_3N_4$ and the PDOS diagrams for (b) $Au_4$, (c) $Ag_4$, (d) $Cu_4$, (e) $Au_2$-$Ag_2$, (f) $Au_2$-$Cu_2$, and (g) $Ag_2$-$Cu_2$/g-$C_3N_4$ complexes (the g-$C_3N_4$ fragment).

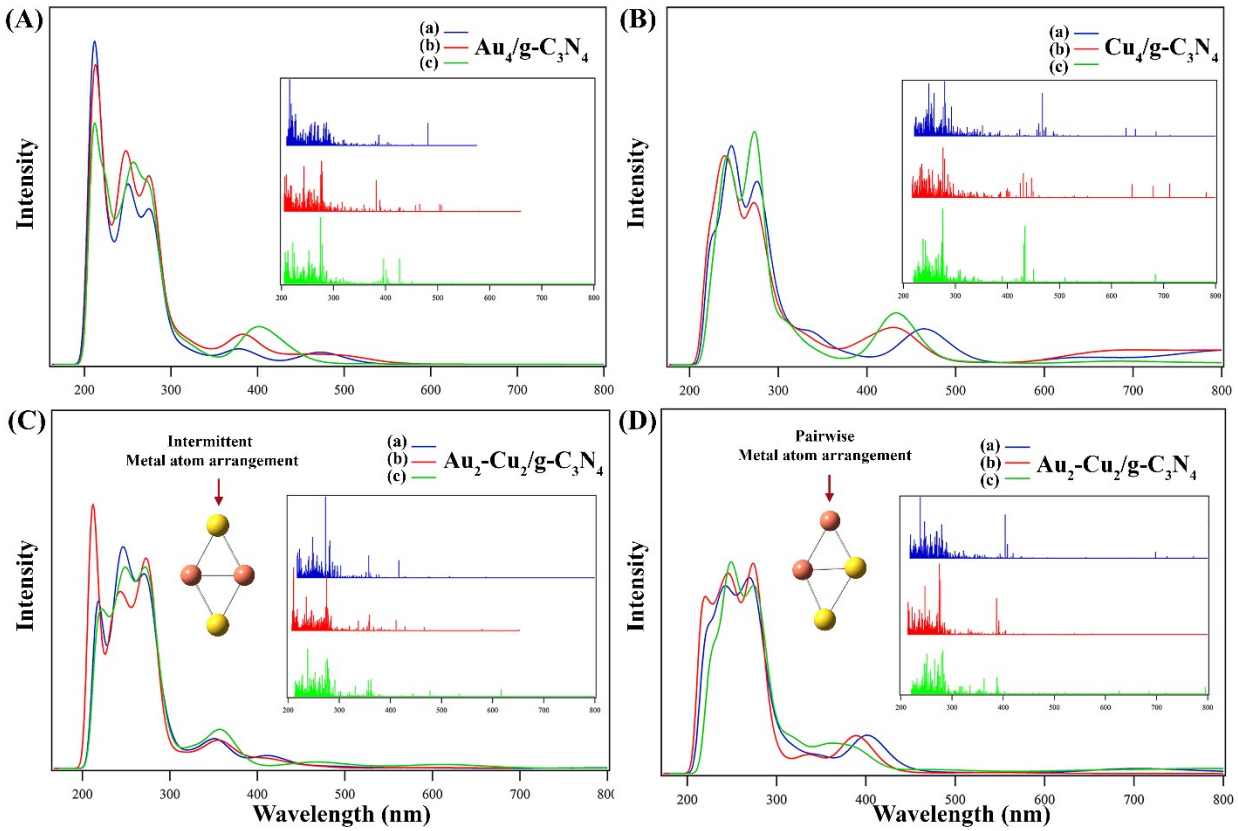


**Fig. S20**. The UV spectra of: (A) $Au_4/g\text{-}C_3N_4$, (B) $Cu_4/g\text{-}C_3N_4$, (C) and (D) $Au_2\text{-}Cu_2/g\text{-}C_3N_4$ with different metal atom arrangements. The interior figures represent the UV absorption lines for each spectrum.

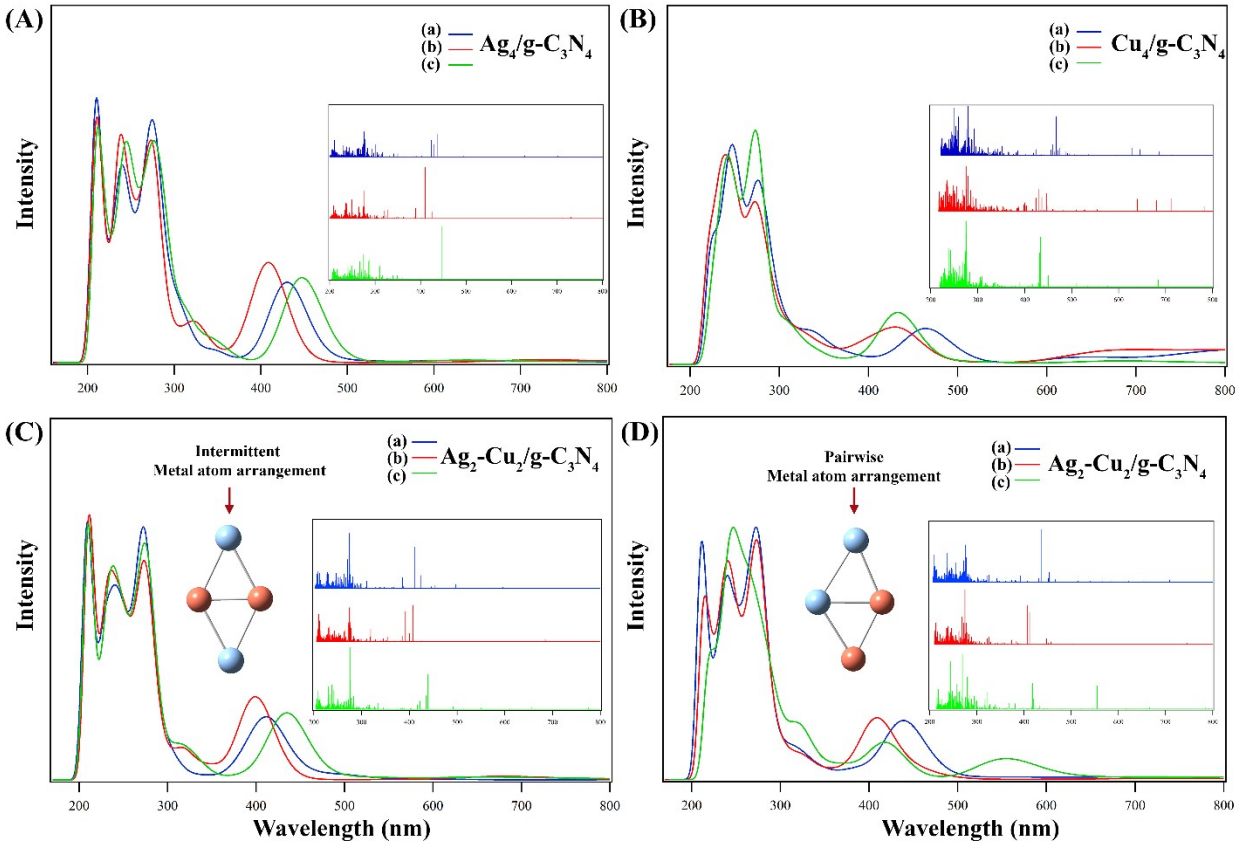


**Fig. S21.** The UV spectra of: (A) $Ag_4/g\text{-}C_3N_4$, (B) $Cu_4/g\text{-}C_3N_4$, (C) and (D) $Ag_2\text{-}Cu_2/g\text{-}C_3N_4$ with different metal atom arrangements. The interior figures represent the UV absorption lines for each spectrum.